OPTIMAL OPERATING TEMPERATURE AND PRESSURE OF PEM FUEL CELL SYSTEMS IN AUTOMOTIVE APPLICATIONS

Bhaskar Balasubramanian, Frano Barbir and Jay Neutzler
Energy Partners, L.C.
1501 Northpoint Parkway
Suite 102, Technology Center
West Palm Beach, FL 33407

INTRODUCTION

The automotive industry is currently faced with the challenge to develop cleaner and energy efficient vehicles in order to meet the reduced toxic emissions standards. The proton exchange membrane (PEM) fuel cell system offers the most promising solution that would enable both efficiency improvement and emissions reduction in automobiles. Since fuel cells use hydrogen as the fuel, in order to facilitate an early market entry, the stacks are being integrated with reformers (fuel processors) that produce hydrogen from conventional fuels such as gasoline, methanol, natural gas, or propane. It is also a viable technology for decentralized power generation. Gasoline being the established vehicle fuel in terms of supply and distribution is best suited for automotive PEM fuel cell system while natural gas is the popular choice for small residential or stationary power applications.

The PEM fuel cell may be operated at pressures ranging from near ambient to about 6 atm and at temperatures between 50 and 90°C. High power density is obtainable at higher operating pressures but the net system efficiency may be lower on account of the power needed for air compression. High power density is also obtained at the higher operating temperatures, however it may pose a significant challenge for water and heat management especially at lower operating pressure. A lower operating temperature, on the other hand, makes waste heat rejection into the environment difficult particularly in hotter surroundings. Therefore selection of operating temperature and pressure of the automotive PEM fuel cell system must be based on (a) high net system efficiency, (b) small component size, and (c) neutral or positive water balance so that the vehicle does not have to carry on-board water reservoir.

In order to select the optimal operating temperature and pressure of the automotive fuel cell system Energy Partners developed a steady-state mathematical model of the entire fuel cell system that estimates the system and component parameters (such as mass flows, reaction rates, heat fluxes and loads, heat exchanger size, component and net system efficiencies etc.) at various operating temperatures and pressures and at various power levels.

SYSTEM DESCRIPTION

As shown in Figure 1, the automotive fuel cell system consists of the following major components or subsystems:

- Fuel Processor (which includes exhaust heat recovery in burner)
- Compressed Air Delivery
- Fuel Cell Stack
- Heat and Water Management
- Exhaust (Expander)

Figure 2 is a 3-D representation of the complete automotive fuel cell system. The fuel to be reformed in this case is gasoline. Epyx Corp.[1] successfully demonstrated a partial oxidation based fuel processor. Gasoline is reformed to produce a reformate stream consisting of approximately 40% hydrogen, 20% carbon dioxide, and balance nitrogen (dry basis) after CO clean-up. A typical reformate stream leaves the fuel processor at near 160-170°C saturated with water vapor. The wet gas is then conditioned to the stack temperature, the condensed water removed in a separator, and sent to the fuel cell anode fully humidified at that temperature. Compressed ambient air is humidified before it is supplied to the cathode. The unutilized/excess hydrogen from the fuel cell anode exhaust is burnt with the excess air (from the cathode exhaust) in the tail gas catalytic combustor (TGC). Exhaust gases from the TGC are then expanded to recover part of the energy needed for compression. In most applications the fuel cell temperature is controlled using water. However, for an automotive system like the one described here, an anti-freeze liquid such as propylene glycol is preferable. Heat from the coolant loop is rejected in an air-cooled heat exchanger or radiator. Water is consumed in the fuel processor in the steam-reforming and shift reactions, and in the humidification of air. In addition water is needed as the cooling medium in the fuel processor Water is produced in the stack as a result of the reaction between H_2 and O_2, and also in the TGC by combusting hydrogen. For an automotive system it is important to have a neutral water balance to avoid on-board de-ionized water supply. Therefore, liquid water is separated from all gas streams (fuel cell exhaust gases and the TGC exhaust) and conditions maintained so as to achieve neutral water balance. The electrical power generated by the fuel cell is used to power the auxiliary loads (compressor/expander, pumps, radiator fan, and control equipment) in addition to that required by the automotive propulsion unit.

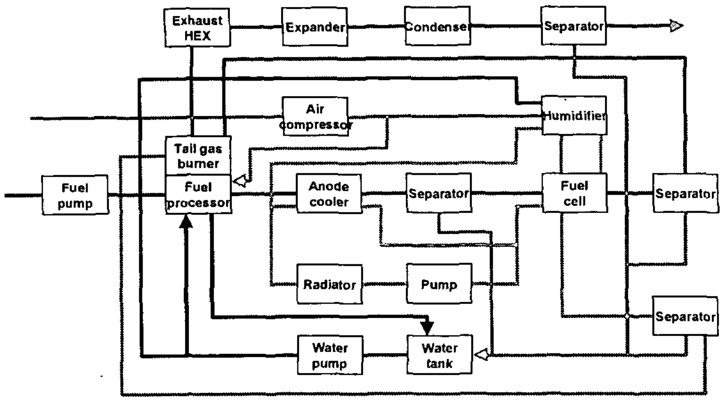

Figure 1. Automotive PEM Fuel Cell System Block Diagram

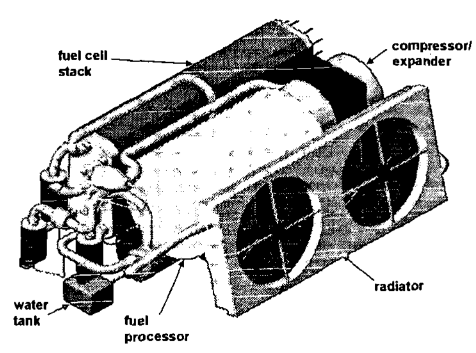

Figure 2. A 3-D Representation of the Automotive PEM Fuel Cell System

MODEL DESCRIPTION

Based on the laws of conservation of mass and energy a complete set of equations was developed to compute mass and energy balance of each species in the system. The model takes into account all the chemical reactions involved in the fuel processor, fuel cell, TGC, etc., and the energy changes associated with the phase change of some of the species due to changes in temperature, pressure, etc.

Fuel Processor:

The fuel processor combines partial oxidation, steam reforming and water gas shift reactions to produce hydrogen, which for gasoline reforming can be represented as:

$C_8H_{18} + (12.5)/\phi\ O_2 + (16 - 25/\phi)\sigma\ H_2O \rightarrow aCO_2 + bCO + cCH_4 + dH_2 + eH_2O$

where:

ϕ = equivalence ratio, (stoichiometric air/fuel ratio to actual air to fuel ratio)

σ = ratio of actual to theoretical H_2O in the fuel processor

The coefficients (of the products and unconverted reactants) are calculated based on the mass balance of each of the species involved in fuel processing. The efficiency of fuel processing is then computed as the ratio of the heating value of product hydrogen to that of gasoline reformed. In order to reduce the CO content to less than 100 ppm (to prevent poisoning of the Pt anode catalyst), CO is further preferentially oxidized (PROX) using air over a special catalyst. Approximately, for 1% of the CO in the reformate and twice the excess oxygen needed, 2.5% of the hydrogen in the reformate is also oxidized resulting in an efficiency of 97.5% for preferential oxidation. Thus based on the amount of hydrogen required, the model calculates the mass flows of the reacting species.

Fuel Cell:

The stoichiometric amounts of H_2 and O_2 consumed in the electrochemical reaction in the fuel cell are computed by Faraday's law. However, since neither H_2 nor O_2 is present as pure gas excess amounts are supplied to the fuel cell and the unused H_2 is burnt with the unused O_2 in the TGC later for heat integration with the reformer. The H_2 stoichiometric ratio depends on the actual fuel cell flow field design. The power generated by the fuel cell stack is a product of the individual cell voltage, current density and the number of cells. The current and voltage are related according to the polarization curve and an experimentally determined curve is used in the model. The fuel cell efficiency is defined as the ratio of the electrical power output to the heating value of H_2 fed.

$$\eta_{FC} = (I \, . \, V_{cell}) \, / \, (\Delta H_{H_2} \, . \, \text{Mass } H_2 \text{ fed})$$

It can thus be seen that high efficiency is obtainable at higher fuel cell potential and lower H_2 stoichiometry. However for any given power output a high fuel cell operating voltage leads to larger stack.

Air Supply and Exhaust Heat Recovery:

Unused H_2 from the fuel cell is combusted in the TGC and the heat generated is utilized in the fuel processor for preheat and/or steam generation. Combustion being exothermic, temperature of the exhaust gases is relatively very high and the heat is utilized in an expander to generate part of the power needed for air compression. It will be explained later that an expander is necessary for a pressurized system. Power recovered in the expander is computed using isentropic equations. Similarly, based on O_2 flow needed for the fuel cell, air flow is computed and compressor is sized accordingly.

Water and Heat Management:

The coolant flow is computed depending upon the heat generated in the fuel cell and the operating temperature. Accordingly, the model calculates the cooling duty needed in the coolant loop and estimates size and other parameters for the radiator.

System Efficiency:

The overall system efficiency is a product of the efficiencies of the fuel processor, the PROX unit, the fuel cell and balance of plant (η_{BOP}). η_{BOP} is the ratio of the net power to the gross power produced by the fuel cell. The difference between gross power and net power includes power needed to run compressor/expander, fans, pumps, solenoid valves, relays, controller, etc.

RESULTS AND DISCUSSION

The model briefly described above was used to perform steady state simulations to calculate the following system parameters (based on the input parameters and assumptions outlined in Table 1): (a). fuel consumption, air and water requirements; (b) fuel cell parameters (size and number of cells); (c) parasitic load requirements or BOP analysis.

Table 1. Input parameters

Net power output:	50 kW
Fuel cell polarization curve:	EP laboratory results
Cell nominal voltage:	Variable
Operating pressure:	Variable from 101.3 to 308 kPa
Operating temperature:	Variable from 50 to 80 °C
Reactants humidification:	both gases 100% RH at operating temp.
Stack ΔT:	10°C
Stack pressure drop:	15 and 30 kPa
Stoichiometry:	2.0 cathode; 1.17 anode
Compressor efficiency:	0.8
Expander efficiency:	0.8
Expander inlet temperature (max):	150°C
Reformer efficiency:	0.8 (LHV)
Reformer fuel equivalence ratio:	3.13
Water/fuel ratio in reformer (mol):	22.84
Fuel:	Octane (C_8H_{18})
PROX stoichiometry:	2 (efficiency 0.97)
Reformer pressure drop:	15 and 30 kPa
Ambient conditions:	101.3 kPa, 30°C, 60%RH

Figure 3 shows the dependence of the system efficiency on fuel cell operating temperature and pressure. For the pressurized system a higher operating temperature results in a somewhat higher system efficiency and vice-versa for a low temperature system, which is mainly due to: (a) at low operating pressure, the expander recovers very less or no power, and (b) high operating temperature when coupled with low pressure necessitates large amounts of water recovery in the condenser which results in a very high parasitic load for the condenser fan. It should be noted that in these comparisons, the fuel cell voltage at nominal power was kept constant at 0.7 V/cell. A higher cell voltage results in higher efficiency but results in less power density (W/cm^2) or in other words a larger stack. Figure 4 shows relative stack sizes as a function of temperature and pressure at constant nominal system efficiency. High temperature and high pressure lead to the smallest stack size.

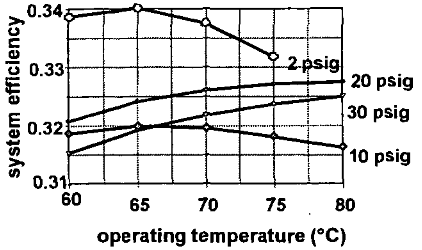

Figure 3. Effect of Operating Temperature and Pressure on System Efficiency

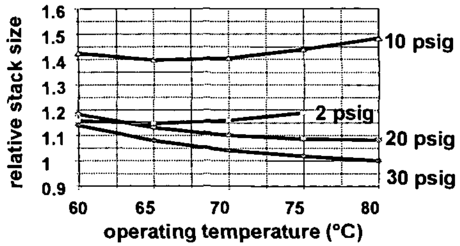

Figure 4. Effect of Operating Temperature and Pressure on Stack Size

However stack size is not the only criteria in selecting operating temperature and pressure. Size and performance of other components such as the fuel processor and radiator are also affected by pressure and temperature. Figure 5 shows the variation in heat load on the condenser and radiator with operating temperature and pressure. High temperature when coupled with low pressure shifts the heat load from the condenser to the radiator. On the other hand, high pressure and low temperature results in maximum heat rejection in the radiator. The major difference between these two components is that the radiator is liquid-to-gas heat exchanger while the condenser is a gas-to-gas heat exchanger. Heat transfer coefficients are significantly lower for the condenser, which means that for a given heat load the condenser requires much larger heat transfer area than the radiator. Figure 6 compares the heat transfer areas for the condenser and radiator as a function of temperature and pressure. The calculations assume a liquid/gas heat transfer coefficient of 60 W/m^2/°C and gas /gas coefficient of 15 W/m^2/°C and a fin-to-tube area of 10. The system that operates at high pressure (30 psig) and low temperature (60°C) requires the smallest heat exchanger. For automotive fuel cell systems heat exchanger size may very well be a limiting factor. At 30 psig and 60°C, there is no need for a condenser since all heat is rejected in the radiator.

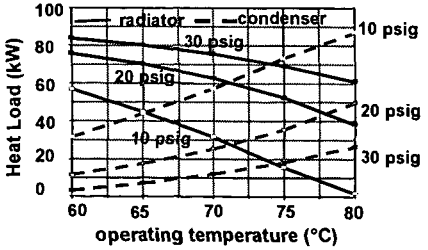

Figure 5. Radiator and Condenser Heat Load (50 kW net, constant efficiency)

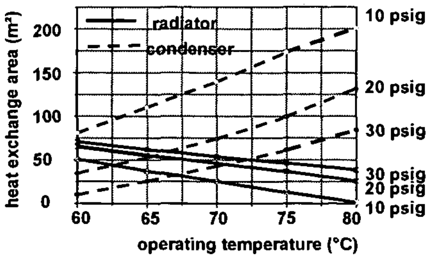

Figure 6. Required Heat Exchanger Area for a 50 kW (net) System

In all cases neutral water balance was accomplished such that enough water was condensed in the system to make up for the reformer process water and for air humidification. Water management poses a concern in systems that operate at low pressures and high temperatures since large amounts of water are needed for humidification.

With certain assumptions and limitations, the model also simulates the performance at off-design conditions such as partial loads and ambient conditions. Figure 7 shows projected system efficiency at various power levels. At 25% net peak power, the net system efficiency is around 39%. However for a realistic case, since the efficiencies of the compressor and expander are lower at lower pressures and lower power levels, the system efficiency is around 37%. Again, higher efficiencies (>40%) are obtainable at higher cell voltages at peak power. Ahluwalia et. al [2] have shown that 44.8% system efficiency is obtainable at 0.8 V/cell and 90% hydrogen utilization.

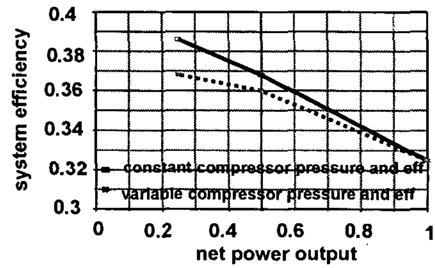

Figure 7. System Efficiency as Function of Net Power Output
(30 psig, 80°C, 50 kW - peak power)

CONCLUSIONS

The numerical steady state model developed for performance simulation of the PEM fuel cell automotive system has proven to be a valuable tool for component sizing, trade-off analysis by varying system configurations, and optimizing system pressure and temperature. Results suggest that an automotive system should operate at high pressure (30 psig), but an expander must be used to recover power used for compression. Surprisingly, results indicate that a low temperature (60°C) results in smallest size of heat exchanger if neutral water balance is mandated. The model also predicts system efficiency at different loads. Higher efficiencies may be achieved at higher cell voltages, but that would result in large fuel cell stack, which may be a limiting factor for automotive applications with the state-of-the-art fuel cells.

ACKNOWLEDGEMENT

This work was supported by the U.S. Department of Energy, Office of Advanced Automotive Technologies, under contract no. DE-FC02-97EE50476.

REFERENCES

1. W.L. Mitchell, "Integrated Power System for Transportation - Advanced Fuel Processor Development", Fuel Cells for Transportation 98, Contractors Annual Progress Report, Vol. 1, pp23-27, U.S. Department of Energy, OAAT, Washington D.C., November 1998.
2. R.K. Ahluwalia, E.D. Doss, H.K. Geyer and R. Kumar, "Pressurized POX-Reformed Gasoline PEFC System", presented at the Pressure Effects Workshop, Argonne National Laboratory, Argonne, IL, December 1998.